

ROTATIONAL SPECTROSCOPIC STUDIES ON THE CH₃CN-CO₂ COMPLEX

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The CH₃CN-CO₂ complex was investigated using a Pulsed-Nozzle Fourier Transform Microwave Spectrometer. This complex offers the possibility of observing a 'carbon-bonded' structure. The ab initio calculations give three minima structures; a π -stacked structure, a T-shaped structure with the N end of CH₃CN interacting with the C atom of CO₂, and a linear structure with the O of CO₂ interacting with the tetrahedral C of CH₃CN. Thus, the T-shaped and the linear structures are bound with a 'carbon-bond'. The π -stacked and T-shaped structures have similar binding energies (-7.7 kJmol⁻¹ and -7.6 kJmol⁻¹, respectively). Many lines were observed which depend on both CH₃CN and CO₂ concentrations. Six of these lines follow a nearly prolate, 'a'-type spectra. The K=0 (J = 3-2 to 8-7) rotational transitions have been observed. The B+C value obtained from fitting these transitions is consistent with the value predicted for the T-shaped geometry with an N-C interaction. All lines show hyperfine splitting due to quadrupole coupling of the nitrogen atom. Measurements with isotopic substitutions have been carried out to ascertain the assignment of the rotational transitions. The unassigned lines may belong to the other possible geometries of the CH₃CN-CO₂ complex.